Three-Dimensional Simulations of the Electrothermal and Terahertz Emission Properties of Bi$_2$Sr$_2$Ca$_2$O$_8$ Intrinsic Josephson Junction Stacks

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We use 2D coupled sine-Gordon equations combined with 3D heat diffusion equations to numerically investigate the thermal and electromagnetic properties of a 250 $\times$ 70 $\mu$m$^2$ intrinsic Josephson junction stack. The 700 junctions are grouped to 20 segments; we assume that in a segment all junctions behave identically. At large input power, a hot spot forms in the stack. Resonant electromagnetic modes oscillating either along the length [(0, $n$) modes] or the width [(m, 0) modes] of the stack or having a more complex structure can be excited both with and without a hot spot. At fixed bath temperature and bias current, several cavity modes can coexist in the absence of a magnetic field. The (1, 0) mode considered to be the most favorable mode for terahertz emission can be stabilized by applying a small magnetic field along the length of the stack. A strong field-induced enhancement of the emission power is also found in experiment for an applied field around 5.9 mT.

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I. INTRODUCTION

Stacks of intrinsic Josephson junctions (IJJs) in the high-temperature superconductor Bi$_2$Sr$_2$Ca$_2$O$_8$ (BSCCO) emit coherent radiation at terahertz frequencies [1]. The emitted frequency $f_e$ follows the Josephson relation $f_e = V_J/\Phi_0$, where $\Phi_0$ is the flux quantum ($\Phi_0^{-1} = 483.6$ GHz/mV), and $V_J$ is the voltage across a single junction. In BSCCO, superconductivity is restricted to $d_s = 0.3$ nm thick CuO$_2$ sheets separated by barrier layers to form an $s = 1.5$ nm thick IJJ [2]. In Ref. [1], stacks of approximately 700 IJJs, with a length $L_s \sim 300$ $\mu$m and a width $W_s$ of some 10 $\mu$m have been realized as mesas on top of BSCCO single crystals. These mesas emitted radiation between 0.35 and 0.85 THz, with an integrated output power of approximately 1 $\mu$W. The emission frequency scaled as $W_s^{-1}$, indicating that cavity modes oscillating along the width of the stack are responsible for synchronization. Terahertz radiation from IJJ stacks became a hot topic both in experiment [3-35] and theory [36–66]; for a recent review, see Ref. [67].

IJJ stacks containing 500–2000 junctions have been patterned as mesas but also as bare IJJ stacks contacted by Au layers (GBG structures) [16,17,20,24] and as all-superconducting structures [11]. Emission frequencies range from 0.3 to 2.4 THz. For the best stacks, an emission power $P_e$ in the range of tens of microwatts has been achieved [17,19,20,32,33], and arrays of mesas showed emission with $P_e$ up to 0.61 mW [19]. The physics of the huge IJJ stacks is affected by Joule heating [1,3,5,6,8,13,18,22,26,30,49,52,54,55,63]. For sufficiently low-bias currents, the temperature rises only slightly to values above the bath temperature $T_{bath}$, and the voltage $V$ across the stack increases with increasing bias current $I$. With increasing $I$ and input power, the current-voltage characteristics (IVCs) start to backbend, and, at some bias current in the backbending region, a hot spot forms in the stack [3,6,8,13,18,21–23,25,26,34,68], creating a region heated to temperatures above the critical temperature $T_c$. Similar effects also occur in other systems [69,70]. The terahertz emission properties of the IJJ stacks are affected by the hot spot. For example, it has been found that the linewidth of radiation is much narrower in the high-bias regime than at low bias [12,60]. Other properties such as the emission frequency seem to be basically independent of the hot-spot position, leading to some debate as to whether the hot spot is helpful for radiation or just coexists with the radiating regions [20,22,23]. In fact, recent results showed that there is a strong interaction [28]. Further, cooling has been improved by sandwiching the stacks between substrates with high thermal conductivity. In the first attempts, maximum emission frequencies near 1.05 THz were obtained [24,68]. This value was recently improved to 2.4 THz for disk-shaped stacks [33]. In terms of modeling, many calculations of electrodynamics have been based on a homogeneous temperature distribution, while calculations of the thermal properties were based on solving the heat diffusion equations in the absence of Josephson
currents [49,52,54]. Some attempts have been made to combine both electrodynamics and thermodynamics, either by using arrays of pointlike IJJs [59,60,64] or by incorporating temperature-induced effects into an effective model describing the whole stack as a single “giant” junction [55,62,63]. Reference [66] modeled the combined thermal and electromagnetic properties of BSCCO stacks via one-dimensional coupled sine-Gordon equations for an $N = 700$ junction stack where the IJJs were grouped into $M$ segments [66].

II. MODEL

The model introduced here extends the 2D approach of Ref. [66] to 3D, enabling us to model IJJ stacks realistically. We first give a brief outline of the features which go beyond Ref. [66]. We consider a mesa consisting of $N = 700$ IJJs; cf. Fig. 1(a). The mesa has a length $L_x = 250 \mu m$ along $x$ and a width $W_y = 70 \mu m$ along $y$. It is covered by a gold layer and centered on a base crystal, which is found by self-consistently solving the heat diffusion equation

$$cT = \nabla(k \nabla T) + q_m + q_b,$$

with the specific heat capacity $c$, the (anisotropic) thermal conductivity $k$, and the power densities $q_m$ and $q_b$ for heat generation in the mesa and the bond wire, respectively. For high enough $q_b$, the hot spot is controllably located near the wire position.

For the electric circuit, we group the $N$ IJJs in the mesa to $M$ segments, each containing $G = N/M$ IJJs, assumed to have identical properties. The bond wire injects an electric current density $j_{\text{ext}}$ to the Au layer, which we assume to have a low enough resistance to freely distribute the current before it enters the IJJ stack in the $z$ direction with a density $j_{z,\text{Au}}$ proportional to the local BSCCO conductance $\sigma_c(x,y) = \rho_c^{-1}(x,y)$. The full expression is

$$j_{z,\text{Au}} = (j_{\text{ext}}) \sigma_i(x,y)/\sigma_c,$$

where $\sigma_i$ denotes the local BSCCO conductance and $\sigma_c$ the critical current density. The z-axis currents consist of Josephson currents with critical current density $j_{\text{c}}(x,y)$, (Ohmic) quasiparticle currents with resistivity $\rho_c(x,y)$, and displacement currents with dielectric constant $\varepsilon$.

To avoid weakly stable solutions, we also add Nyquist noise created by the quasiparticle currents. The in-plane currents consist of a superconducting part characterized by a Cooper pair density $n_c(x,y)$, a quasiparticle component with resistivity $\rho_{ab}(x,y)$, and a Nyquist noise component. For constant $T_m(x,y)$, we index the above quantities by an additional “0” and assume that they are constant with respect to $x$ and $y$. The temperature dependence of the various parameters is close to experimental curves and plotted in detail in Ref. [66]. We further use $T_c = 85$ K.

One obtains sine-Gordon-like equations for the Josephson phase differences $\gamma_m(x,y)$ in the $m$th segment of the IJJ stack:

$$Gsd_i \nabla \left( \frac{\nabla \gamma_m}{\rho_{ab}} \right) + d_i \nabla (j_{x,m}^N - j_{m}^N) + G \frac{\lambda_c}{\rho_{ab}} \nabla (n_c \nabla \gamma_m) = 2 J_{z,m} - J_{z,m+1} - J_{z,m-1}.$$

Here, $m = 1, \ldots, M$, $\nabla = (\partial/\partial x, \partial/\partial y)$, and $\lambda_c = |\Phi_0|d_i/(2\pi \mu_0 \rho_{ab}^0)^{1/2}$, with the in-plane London penetration depth $\lambda_{ab0}$ and the magnetic permeability $\mu_0$. Quantities $j_{x,m}$ are the in-plane noise current densities. Time is normalized to $T_\text{c}$, laser power density $W_l$, and the magnetic field $\Phi_0 = 2\pi j_{\text{c}} \rho_{ab}^0 \varepsilon_0$. Resistivities to $\rho_{ab}$, and current densities to $j_{\text{c}}$.

Equation (2) neglects geometric inductances; i.e., it assumes that kinetic inductances dominate (valid if $L_x$, $W_y < \lambda_c$; $\lambda_c \sim 300 \mu m$ is the out-of-plane penetration depth).

For the out-of-plane current densities $j_{z,m}$, one finds

$$j_{z,m} = \beta_{e0} \gamma_m + \frac{j_m}{\rho_{e,c}} + j_c \sin(\gamma_m) + j_{c,m}^N,$$

with $\beta_{e0} = 2\pi j_{\text{c}} \rho_{ab}^0 \varepsilon_0 \Phi_0/\Phi_0$, $\varepsilon_0$ is the vacuum permittivity, and the $j_{c,m}^N$ are the out-of-plane noise current densities.
From the gauge-invariant Josephson phase differences $\gamma_m$, as calculated from Eqs. (2) and (3), we obtain the phase $\phi_m$ of the superconducting wave function in electrodes $m$ (the CuO$_2$ layer interfacing segments $m$ and $m+1$) via

$$\nabla \gamma_m = \frac{2\pi s}{\Phi_0} (B_{y,m}, -B_{x,m}) + \frac{\nabla(\phi_{m+1} - \phi_m)}{G}. \quad (4)$$

Here, $B_{x,m}$ and $B_{y,m}$ are, respectively, the $x$ and $y$ components of the magnetic field in the $m$th segment.

The in-plane supercurrent densities in units of $j_{c0}$, $\vec{j}^s_m = (j^s_{x,m}, j^s_{y,m})$, in electrode $m$ are expressed as

$$\vec{j}_m^s = \frac{\lambda_m^2 n_s}{d_s} \left( \nabla \phi_m - \frac{2\pi}{\Phi_0} A_m \right). \quad (5)$$

$\vec{A}_m = (A_{x,m}, A_{y,m})$ denotes the in-plane components of the vector potential in electrode $m$. The resistive currents $\vec{j}_m = (j^r_{x,m}, j^r_{y,m})$ in electrode $m$ are given by

$$\vec{j}_m^r = \frac{s}{\rho_{ab}} \frac{d}{dt} \left( \nabla \phi_m - \frac{2\pi}{\Phi_0} \vec{A}_m \right). \quad (6)$$

In our calculations, we assume that the $z$ components of curl$\vec{j}^s_m$ and of curl$\vec{j}^r_m$ vanish, and, thus, inside the superconducting layers, the total magnetic field in the $z$ direction is zero.

For the thermal parameters, we use the same values as in Ref. [66]. The bond wire with resistivity $\rho_b = 0.02 \rho_{c0}$ is assumed to be a $25$-$\mu$m-wide square located at the left edge of the mesa. Further, $\rho_{c0} = 10^3 \Omega \cdot \text{cm}$, $\rho_{ab0} = 8 \mu\Omega \cdot \text{cm}$, $j_{c0} = 200 \text{ A/cm}^2$, $\lambda_{ab0} = 260 \text{ nm}$, and $\epsilon = 12$. For our geometry, one obtains a critical current $I_{c0} = 35 \text{ mA}$, a $c$-axis resistance per junction $R_{c0} = 0.86 \Omega$, a characteristic voltage $V_{c0} = I_{c0} R_{c0} = 30 \text{ mV}$, and a characteristic frequency $f_{c0} = I_{c0} R_{c0} / \phi_0 = 14.5 \text{ THz}$. The characteristic power density $p_{c0} = f_{c0}^2 \rho_{c0}$ is $4 \times 10^7 \text{ W/cm}^3$, yielding for a stack volume of $1.84 \times 10^{-8} \text{ cm}^3$ a power $P_{c0}$ of $0.74 \text{ W}$. For $\lambda_m$, one obtains $0.76 \mu\text{m}$. The $4.2 \text{ K}$ value of the in-phase mode velocity $c_1 = 8.8 \times 10^7 \text{ m/s}$ [66]. We keep the product $\beta_{c0} G$ constant in order to (approximately) fix the $4.2 \text{ K}$ value of $c_1$ and use $\beta_{c0} = 4000$ for $G = 35$ ($M = 20$). We further divide ac electric fields and in-plane current densities by $G$ to make the results only weakly dependent on $M$. For selected bias conditions, the scaling is tested using $M = 50$.

The differential equations are discretized using $50 \times 9$ grid points along $x$ ($y$) for the mesa and $100 \times 18$ grid points for the base crystal [71], which is split into $K = 4$ segments. A fifth-order Runge-Kutta scheme is used to evolve these equations in time. After some initialization steps [66], various quantities partially averaged over spatial coordinates are tracked as a function of time to produce time averages or to make Fourier transforms.

III. RESULTS

Figure 2 shows for $T_{\text{bath}} = 20 \text{ K}$ the averaged distributions of the power density $\langle q_0(x,y) \rangle$ dissipated by in-plane currents for five values of $I/I_{c0} = 0.65$ Fig. 2(a) to 0.1 Fig. 2(e). Averaging is over time and the $z$ direction in the mesa. This type of plot, also used in Ref. [66], is useful to visualize resonance patterns, with nodes (antinodes) appearing at the minima (maxima) of $\langle q_0(x,y) \rangle$ [72]. The left (right) graphs are at high (low) bias where a hot spot is present (absent). In Figs. 2(a) and 2(e), the modulations along $x$ are due to a cavity mode oscillating along $x$ [a $(0,n)$ mode], with $n = 2$ and 3, respectively. In Fig. 2(c), a cavity mode oscillating along $y$ is excited [a $(1,0)$ mode]. The spatial variations in Figs. 2(b) and 2(d) have a more complicated structure which is not easy to explain by a superposition of different cavity modes. The patterns also show that “linear thinking” in terms of separating ac Josephson currents and resonant modes can be dangerous.

Near the antinodes of the standing waves, vortex-antivortex pairs oscillate back and forth, colliding at the center of the antinode [66]. The collision zones should form a continuous line leaving the stack either at its edges or into the hot-spot area. All patterns fulfill this requirement.

In general, not all segments in the stack are synchronized. We investigate this by monitoring the dc voltages ($\alpha$ Josephson oscillation frequency $f_J$) $v_m (m = 1, \ldots, M)$ across the individual segments. For example, for the modes of Figs. 2(a)–2(c), for the two to three uppermost segments, $v_m$ is about 1% higher than for the other (locked) segments. For the mode of Fig. 2(d), only small groups of two to five adjacent segments are locked. For the mode of Fig. 2(e), two groups of segments (one to seven and 10–20) oscillated at slightly different frequencies.

Note that $\langle q_0(x,y) \rangle$ can have similar values for the $(0,n)$ and $(1,0)$ modes; compare, e.g., Figs. 2(a) and 2(c). We expect that both types of modes radiate. However, for comparable values of $\langle q_0(x,y) \rangle$, the emission power of the $(0,n)$ modes, with $n > 1$, will be lower, because the contributions of the oscillating (in-plane) currents to the magnetic vector potential partially cancel each other.

![FIG. 2. Power density $\langle q_0(x,y) \rangle$ in units of $10^{-3} \times f_{c0}^2 \rho_{c0}$ (color scale) for five values of normalized bias current $I/I_{c0}$ (upper left numbers); values for $k_{\text{max}}$ at the bottom left. The gray square in (a) indicates the position of the bond wire. Regions enclosed by the black line are at $T_m \geq T_c$.](image-url)
For each value of $I$ and $T_{\text{bath}}$, we evaluate the type of mode by inspecting the plots as in Fig. 2 and encode it as the shape of the symbol in Fig. 3(a). To have a measure of the strength of a given mode, we record time traces $q(f)$ of the power generated by in-plane currents, averaged over the stack volume. After Fourier transform, we extract from $q(f)$ the power density $q(f)$ arising from the Josephson oscillations appearing as a peak at twice the Josephson frequency $f_J$. This quantity is plotted as the color scale for each data point. In Fig. 3(a), there are three regions where $q(f)$ is low: (i) for $I/I_{c0} > 0.5$ and $T_{\text{bath}} > 55$ K, (ii) for $T_{\text{bath}}$ around 35 K and $I/I_{c0} > 0.65$, and (iii) for $V/NV_{c0} > 0.06$. In region (i), no or only a small fraction of the stack is superconducting; Josephson oscillations are absent or restricted to a small area. In region (ii) the in-plane and out-of-plane currents exhibit short-wavelength oscillations along $x$ and $y$, indicative of a mode with spatial variations shorter than our grid spacing. The spectrum of $q(f)$ is broad, with no significant peaks. In region (iii), where $V$ and $f_J$ are highest, all currents and fields vary smoothly, but no resonance is excited. In the presence of a hot spot [data points at or above the black line in Fig. 3(a)], $q(f)$ is large in a ribbon between $V/NV_{c0} \sim 0.025$ and 0.05. This regime extends down to approximately 0.02 in the low-bias regime. The relative broadness of this regime may look surprising, since resonant modes are excited; however, it can be understood from the facts that the mode velocities depend on the temperature and vary significantly over the data points in Fig. 3(a). Also, the quality factor of the cavity modes is low (of order 10) at elevated temperatures. Most important, one notes that $(0,n)$, $(1,0)$, and mixed modes vary almost randomly. Further simulations reveal that even for the same value of $I$ and $T_{\text{bath}}$, different resonant modes can be excited. However, it should be possible to support the $(1,0)$ mode favored for radiation by applying a small static magnetic field along $x$, imprinting a linear phase gradient and, consequently, a small gradient on the Josephson current around $35$ K and $I_{c0}$. We also test experimentally the potential benefit of a small magnetic field oriented along $x$, using a $75 \times 330$ $\mu$m$^2$ large GBG structure with $N \approx 760$, mounted on a sapphire lens. Figure 4 shows for (a) $B_x = 0$ and (b) $B_z = 5.9$ mT ($0.32 V_{c0}$ per junction) families of IVCs measured for $10$ K $\leq T_{\text{bath}} \leq 45$ K. IVCs at 0 and 5.9 mT are measured alternately at given $T_{\text{bath}}$. The accuracy in aligning the field with respect to out-of-plane tilts is better than 0.5°, and with respect to in-plane tilts, it is about 2°.

The simultaneously detected terahertz emission power $P_e$ measured via a Ge bolometer is plotted as a color scale. In the high-bias regime, the maximum emission power $P_{e,\text{max}}$ is 27.5 $\mu$W, while at low bias, it is 0.21 $\mu$W. We, thus, use different values for $P_{e,\text{max}}$ for $I > 8$ mA and for $I < 8$ mA; for fixed $I$, $P_{e,\text{max}}$ is the same in Figs. 4(a) and 4(b). For $B_x = 0$, the emission is strong for $I$ between 10 and 20 mA and $T_{\text{bath}}$ between 10 and 40 K. One notes short-period oscillations in $P_e$ which presumably are extrinsic in origin. These oscillations have been observed before [28,35,66].

Apart from that, the plots clearly show that for $B_z = 5.9$ mT, over a wide range of currents and bath temperatures, $P_e$ increases significantly in some of the striplike regions up to a factor of 2.7. In the low-bias
In Ref. [73], a 20% increase of on a much lower level of regime, the effect is seen even more drastically, although on a much lower level of $P_{e,\text{max}}$. The idea of applying a small field parallel to the long side of the stack, as suggested by the simulations, thus, seems to work. For other field orientations, the effect is not observed. Even a small field component perpendicular to the layers strongly suppresses orientations, the effect is not observed. Even a small field parallel to the long side of the stack, as suggested by the simulations, thus, seems to work. For other field orientations, the effect is not observed. Even a small field parallel to the long side of the stack, as suggested by the simulations, thus, seems to work. For other field orientations, the effect is not observed. Even a small field parallel to the long side of the stack, as suggested by the simulations, thus, seems to work. For other field orientations, the effect is not observed.

FIG. 4. Experimental data for a GBG structure: terahertz emission power $P_e$ (color scale) for a large number of IVCs, measured at bath temperatures between 10 and 45 K for (a) $B_x = 0$ and (b) $B_x = 5.9$ mT. In both (a) and (b) $P_{e,\text{max}} = 27.5 \mu W$ for $I > 8$ mA and $P_{e,\text{max}} = 0.21 \mu W$ for $I < 8$ mA. Black lines in (a) and (b) indicate the $T_c$ line.

A 20% increase of $P_e$ is observed for fields oriented in the $a$-$b$ plane. Unfortunately, the field direction relative to the mesa edges is not reported.

V. SUMMARY

In summary, we present 3D simulations of the thermal and electromagnetic properties of a mesa consisting of 700 intrinsic junctions. Resonant modes can be excited in the stack both in the presence and in the absence of a hot spot, exhibiting standing waves either along the length or width of the stack. Also, more complex mixed modes are found. At fixed bath temperature and bias current, different modes can coexist. By applying a small magnetic field along the length of the stack, it is possible to stabilize the $(1,0)$ mode considered to be the best mode for terahertz emission. In experiment, we find a strong field-induced enhancement of the emission power for a stand-alone stack for fields of around 5.9 mT, small enough to be created by a simple electromagnet.

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[71] Note that for $M = 20$ and the relatively low number of grid points along $x$ and $y$, we cannot resolve modes that fluctuate strongly in space, like antiphase oscillations of different junctions or static triangular fluxon lattices appearing in magnetic fields on the order of a flux quantum per junction. However, we are mainly interested in dynamic in-phase solutions which can be captured well with the discretization used.

[72] A perhaps more natural choice is to look at the time average $\langle E_z^2(x, y) \rangle$ of the square of the $z$-axis electric fields. However, $E_z(x, y, z, t)$ has a large dc component, and features of oscillating standing waves are only weakly visible.